

CHEMICAL PROCUREMENT TRACKING

Purpose This Air Quality Group procedure describes the process for reviewing and evaluating chemical procurement records as a method of identifying and quantifying regulated chemicals.

Scope This procedure applies, when referred from another procedure, to the identification and quantification of regulated chemicals purchased and used at LANL, including Hazardous Air Pollutants (HAPs); Volatile Organic Compounds (VOCs); 112r Chemicals; SARA 313 Toxic Chemicals; and Toxic Air Pollutants (TAPs). This procedure is not intended to describe the requirements nor to instruct on compliance with the various rules and regulations.

In this procedure This procedure addresses the following major topics:

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Signatures

Prepared by: _____ Jackie Hurtle, ESH-17	Date: <u>1/12/98</u>
Approved by: _____ Leland Maez, SARA 313 Project Leader	Date: <u>1/12/98</u>
Approved by: _____ Steve Story, Operating Permit Project Leader	Date: <u>1/13/98</u>
Approved by: _____ Terry Morgan, QA Officer	Date: <u>1/20/98</u>
Approved by: _____ Doug Stavert, ESH-17 Group Leader	Date: <u>1/20/98</u>

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General information about this procedure

Attachments This procedure has no attachments.

History of revision This table lists the revision history and effective dates of this procedure.

Revision	Date	Description Of Changes
0	1/20/98	New document.

Who requires training to this procedure? The following personnel require training before implementing this procedure:

- individuals assigned to track (for air quality compliance reporting) regulated chemicals procured and used at LANL

Training method The training method for this procedure is on-the-job training by a previously-trained individual and is documented in accordance with the procedure for training (ESH-17-024).

Definitions specific to this procedure CAS numbers: Chemical Abstracts Service number that identifies chemicals.

References The following documents are referenced in this procedure:

- ESH-17-024, "Personnel Training"

Note Actions specified within this procedure, unless preceded with "should" or "may," are to be considered mandatory guidance (i.e., "shall").

Obtaining chemical procurement data

Primary source of data

The Automated Chemical Inventory System (ACIS) is the most comprehensive source of procurement records and is a good starting point for the identification of hazardous chemicals purchased by LANL. ESH-5 can provide the data and help to identify the weaknesses and suggest methods or resources to compensate for the weaknesses.

Overcoming data gaps

Supplemental data should be used when they are available and when ACIS deficiencies are identified.

Pull data together from additional sources, including but not limited to:

- STORES database (primarily gases)
 - project managers (primarily large purchases)
 - new project reviews (primarily large purchases)
 - orders tracked by BUS Division (primarily large purchases)
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Obtain chemical procurement data

ACIS and STORES data are available from ESH-5 and should be requested for a specific span of time. The data should include but are not limited to the following: material name, CAS number, amount, unit of measure, and TA and building number. (The CAS number is not always available.) Supplement these data as necessary and as suggested above.

Obtain regulated chemical lists

Obtain or maintain electronic lists of regulated chemicals by CAS number. The lists of regulated chemicals may change periodically. Ensure that the most up-to-date lists are used for this evaluation. These lists can be located in EPA documents, on the regulatory agencies' Internet web pages, or from other reliable resources. These lists may include HAPs, VOCs, 112r, SARA 313, TAPs or other chemical lists requiring demonstration of compliance or determination of applicability.

Processing and evaluating chemical data

Compile electronic files

Import the electronic files containing the data (obtained as described in the previous chapter) into a spreadsheet or database. These files should include the chemical data and regulated chemicals lists. Supporting files may include composition information, concentration, and specific gravities listed by CAS numbers. If available, use commercial files for the composition information and specific gravities. Otherwise, use best available data (e.g., MSDSs or other chemical references).

Steps to quantify and characterize materials without CAS numbers

To characterize materials without CAS numbers, perform the following steps:

Step	Action
1	Select from the chemical data the materials that are listed without CAS numbers. This group of chemicals consists mainly of mixtures.
2	Convert the quantities to pounds. For the conversion of liquid volumes to mass, assume a specific gravity of 1. For the conversion of gas volumes to mass, use the ideal gas law at standard temperature (20° C) and pressure (1 atm).
3	Rank the totals of each chemical.
4	Select the chemical with the largest total. Locate material data from commercial files, MSDSs, or other chemical references. Identify the constituents, the percent of composition, CAS numbers for constituents, and specific gravity of the material. Add this data to the electronic files.
5	Repeat step 4 until the time and effort for characterization of the next chemical outweighs the benefit (i.e., when the characterization of top-ranking chemicals fails to significantly reduce the total quantity of the materials missing CAS numbers) or until the chemical quantities have been characterized below a statutory threshold.
6	Document the remaining total number of pounds that describes the materials without CAS numbers.

Processing and evaluating chemical data, continued

Steps to quantify and characterize materials with CAS numbers

To characterize materials with CAS numbers, perform the following steps:

Step	Action
1	Select from the chemical data the materials that are listed with CAS numbers.
2	For this group of chemicals, convert the quantities to pounds. For the conversion of liquid volumes to mass, assume a specific gravity of 1 if actual data are not available. For the conversion of gas volumes to mass, use the ideal gas law at standard temperature (20° C) and pressure (1 atm).
3	Rank the totals of each chemical.
4	Select the chemical with the largest total. Locate material data from MSDSs or other chemical reference. Identify the specific gravity of the material. Add this value to the electronic files.
5	Repeat step 4 until the time and effort for characterization of the next chemical outweighs the added benefit or until the chemical quantities have been characterized below a statutory threshold.
6	For liquids, recalculate the conversions to pounds by using the actual chemical formulations and specific gravities.

Identify regulated materials

Electronically compare the chemical data with a list of regulated chemicals to identify the regulated materials and their corresponding quantities that are purchased at LANL. Use the CAS number as the link between the two data sets.

Refine the data

After the above steps, the chemical data of interest have been isolated from a large amount of data. It is possible to focus and refine the data to meet the specific reporting requirements of the applicable rule or regulation as specified in the referring procedure.

Document the work

Document the process assumptions that were used when this procedure was followed. Document any steps that were not followed or other deviations from the specified process. The level of documentation should be sufficient to demonstrate compliance with the applicable regulation and to allow duplication of the process.

Records resulting from this procedure

Records

The following records generated as a result of this procedure are to be submitted **as specified in the referring procedure** as records to the records coordinator:

- chemical data results of the evaluation
- assumptions made in the evaluation
- limitations of the data
- annotated process description and list of deviations and assumptions, as appropriate, that will allow duplication of the process

